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Investigation of complex formation between hydroxyapatite and fragments of collagen by NMR spectroscopy and quantum-chemical modeling

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Abstract

The mechanisms of interaction of collagen and hydroxyapatite are of scientific and practical interest, but they are still not established clearly. Based on the results of experimental NMR investigations of the collagen and hydroxyapatite water suspensions it was shown that hydroxyapatite can form the intermolecular complexes with collagen fragments by the interaction of calcium ions with proline group. The results of DFT quantum-chemical calculations of electron and spatial structure of model compounds allowed us to confirm the hypothesis that calcium ion forms weak intermolecular bonds with the oxygen atoms of proline.

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Keywords

Collagen, Density functional theory, Hydroxyapatite, NMR, Quantum-chemical calculations